3-Methylindene

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767-60)-2	DT	XS	ID4	022749

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 2.97

Global applicability domain: Inside

Local applicability domain index: 6.00e-01

Confidence level: 7.67e-01

Nearest Neighbors from the Training Set

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Benzene, (2-chloroethyl)-

Measured: 2.95 **Predicted:** 2.90

Image not found

2-Fluorobenzyl chloride

Measured: 2.67 Predicted: 2.91

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Indan

Measured: 3.18 Predicted: 2.98